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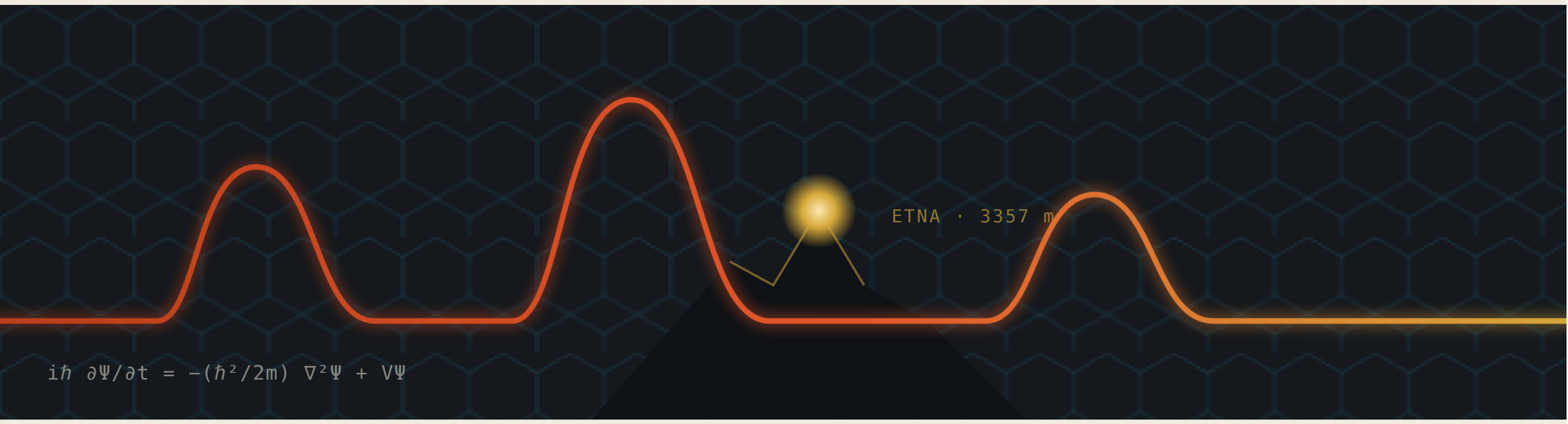
Mathematics, Physics and Technology

Charge Transport, Nonlinear Waves and Mathematical Modeling

◆ BOOK OF ABSTRACTS

Special session dedicated to the scientific activity of **Prof. Vittorio Romano**



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List of Speakers

Multiscale derivation of a coupled charge transport and Helmholtz model from Maxwell's equations

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We present a multiscale derivation of mathematical model for the description of a semiconductor laser diode, starting from Maxwell's equations. The model consists of drift-diffusion equations for the semiconductor variables, coupled with Helmholtz equations for the optical component of the electro-magnetic field. The novelty of this presentation does not lay in the final model, which has been used for years in laser research [1], but rather on the mathematics-oriented approach used in its derivation. Existence and uniqueness of the drift-diffusion/Helmholtz equations have been studied in [2].

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WKB approximation of the fourth order Schrödinger equation in the oscillatory regime

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The fourth order Schrödinger equation (SE4) has been recently introduced in *G.E. Aliffi, G. Nastasi, V. Romano, Z. Angew. Math. Phys., 76:155 (2025)* to describe carrier transport in semiconductor devices, such as resonant tunneling diodes (RTD), when high electric fields are applied and as a consequence when the parabolic band approximation is no longer valid. As for the standard Schrödinger equation, the solutions of the SE4 are highly oscillating, requiring specific numerical techniques for an efficient resolution. In this paper, we adapt a Wentzel–Kramers–Brillouin (WKB) based numerical method, originally developed for the resolution of the standard Schrödinger equation in *A. Arnold, N. Ben Abdallah, C. Negulescu, SIAM Journal on Numerical Analysis, 49(4) (2011)*, to the fourth-order setting. The efficiency of the proposed approach is then assessed through a comparison with a classical finite-difference method, with particular emphasis on accuracy and computational cost.

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Second order unfitted ghost-FEM for elliptic interface problems with applications to low-dimensional semiconductor devices

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We develop an unfitted ghost finite element method for elliptic interface problems with discontinuous diffusion coefficients and apply it to the electrostatic simulation of low-dimensional semiconductor devices. The proposed approach is based on a fixed Cartesian grid and represents the geometry by level-set functions, avoiding mesh generation and remeshing even in the presence of interfaces. A snapping-back-to-grid strategy is used to control the small-cut-cell issue, while interface conditions are weakly enforced by a symmetric Nitsche formulation. The method is first validated on benchmark elliptic interface problems with different geometries and coefficient jumps, showing second-order accuracy for the solution and first-order accuracy for its gradient.

As an application, we consider a graphene field-effect transistor described by a self-consistent drift-diffusion-Poisson model. The electrostatic potential is computed in a two-dimensional oxide/graphene/oxide structure, while charge transport in the graphene layer is modeled by one-dimensional bipolar drift-diffusion equations in the degenerate case and by including a field-dependent mobility model. The coupled nonlinear system is solved by a damped fixed-point iteration combined with a domain-decomposition treatment of the three-layer geometry. Numerical simulations reproduce transfer characteristics with a clear transition from an OFF state to an ON state and show the influence of the gate voltage on the two-dimensional electrostatic potential. The results also indicate that the effective thickness and discretization of the graphene layer affect the transverse potential profile, supporting the use of a full two-dimensional electrostatic description with explicit oxide/graphene interface conditions.

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Heisenberg-like dynamics for non-Hermitian Hamiltonians: some results

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We review some recent results on non-Hermitian Hamiltonians and on their Heisenberg-like evolution, both at a finite and at an infinitesimal level. We particularly focus on conserved quantities and on the spatiality of the algebraic derivation.

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Multiple delta interactions in a bounded domain: spectral analysis and applications

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We investigate a quantum Hamiltonian whose potential is a linear combination of N delta interactions on a bounded interval. A rigorous realization of the Hamiltonian is constructed within the framework of self-adjoint extension theory, starting from an appropriate symmetric operator. Although this class of operators is well understood on the whole real line [1], its extension to a finite domain displays distinctive spectral features. In particular, we discuss conditions under which bound states may fail to exist even for attractive interactions, in contrast with the standard situation on the real line. We also derive an explicit representation of the eigenfunctions associated with the positive spectrum. Besides their theoretical interest, these results may provide useful tools for numerical computations [2]. A possible application concerns the simulation of particle–environment interactions, in which the environment is modelled by N spinors located at fixed positions [1]. The explicit spectral characterization obtained here may facilitate both the analytical study and the numerical implementation of such models.

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Generalized Quantum Observables and their Characterization

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Moving beyond standard projection-valued measures, positive operator-valued measures (POVMs) play a central role in quantum physics, where they provide the mathematical framework for generalized observables, as well as in applications such as signal processing, quantum estimation, and optimal control. We present recent results concerning the existence of Radon–Nikodym derivatives for POVMs with respect to scalar measures, and discuss their mathematical and physical significance. We then turn to the role of POVMs in the foundations of quantum mechanics, showing that they provide a natural framework for the analysis of quantum fuzziness. In particular, we address the open problem of characterizing intrinsic fuzziness, namely the extent to which fuzziness should be regarded as an irreducible feature of quantum systems rather than as a consequence of measurement imperfections or limitations.

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Recent results on thermo-elasticity for beams

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In recent years, increasing attention has been turned to the analysis of some classical engineering structures describing the dynamics of linear and nonlinear vibrations of beams. In the literature, the mechanical properties and the global analysis of the longtime dynamics of axially loaded single beams and of elastically connected double-beam systems were first analyzed within the Euler–Bernoulli theory, also according to the nonlinear Woinowsky–Krieger model [1]. As it is well known, the Euler–Bernoulli beam model wholly ignores the shearing deformation and rotational inertia effects. These limitations require a better-adapted beam model, such as the Timoshenko theory, which seems to have a wider range of applicability and to be physically more realistic since it better captures the behavior of the system [2]. The Timoshenko model is obtained in the particular case where the longitudinal displacement is not considered and by supposing zero initial curvature; thus, it can be generalized by the Bresse system, the governing model for arched beams [3]. These distinct models will be investigated in the context of single and double beams with different dissipative mechanisms in order to obtain their stabilization. A rigorous mathematical investigation of these beam configurations requires, as a fundamental step, a comprehensive analysis of their well-posedness and long-time dynamics [4, 5]. Well-posedness, meaning the existence, uniqueness, and regularity of the solutions, can be established by implementing advanced functional analysis techniques, such as the semigroup theory of linear operators for linear problems, or the Faedo–Galerkin approximation scheme combined with energy methods for nonlinear models. The asymptotic behavior of the thermoelastic and viscoelastic structures as time tends to infinity is investigated by tracking the evolution of the total energy functional. A crucial aspect of this qualitative analysis is to identify the precise rates of energy dissipation. Specifically, it is interesting to determine the exact structural or physical conditions, such as the equality of wave propagation speeds or the geometric coupling coefficients, that trigger a rapid exponential decay of the solutions.

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Reservoir Computing for Scientific Modeling and Data Analysis

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A survey of reservoir computing (RC) as a dynamical framework for learning, classification, prediction, and data analysis is presented.

Two reservoir architectures are considered: the echo-state network and a FitzHugh-Nagumo excitable network, which are implemented to perform tasks of increasing complexity: learning logical functions, physics-informed RC and rollout, image classification with an untrained CNN front-end, and multi-input RC for CLIP-style problems.

The second part of the talk explores how RC can reproduce some biological capabilities of a cerebral microcircuit. In particular, the construction of a bio-inspired sparse RC architecture and an anchor-proximal windowed readout for temporal decision making is illustrated.

Achronal Localization and Representation of the Causal Logic from Conserved Currents

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In this seminar, I will present and discuss recent achievements [1, 2, 3, 4] concerning the theory of achronal localization derived from conserved currents, as well as the representation theory of the Causal Logic of Minkowski spacetime. Due to the one-to-one correspondence between (covariant) achronal localizations and (covariant) representations of the causal logic thus, apparently for the first time, a covariant representation of the causal logic for an elementary relativistic quantum mechanical system has been achieved. Localizations are gained out of covariant conserved currents computing their flux passing through achronal surfaces. This general method applies to the probability density currents with causal kernel regarding the massive scalar boson. Similarly one derives the covariant family of representations of the causal logic related to the stress energy tensor of the massive scalar boson. To prove these results, it is necessary to develop certain techniques of geometric measure theory concerning sets with almost Lipschitz boundaries.

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An existence result in annular regions times conical shells and its application to nonlinear Poisson systems

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We provide a new existence result for abstract nonlinear operator systems in normed spaces, by means of topological methods. The solution is located within the product of annular regions and conical shells. The theoretical result possesses a wide range of applicability, which, for concreteness, we illustrate in the context of systems of nonlinear Poisson equations subject to homogeneous Dirichlet boundary conditions. For the latter problem we obtain existence and localization of solutions having all components nontrivial. This is also illustrated with an explicit example in which we also furnish a numerically approximated solution, consistent with the theoretical results. We conclude with an application of our results to a reaction–diffusion Lotka–Volterra system with source terms for competing species.

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On Leray's théorème de structure for a weak solution to the Navier-Stokes equations: an improvement of the result

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It is well known that for the 3D-Navier-Stokes equations the existence of a global regular solution is not known. We supply to the quoted open question by furnishing a theorem of existence of weak solutions. In accord with Newtonian point of view, Leray (1934) in his paper investigated about the regularity of the weak solution. He furnished the so called *théorème de structure.* The theorem, beyond the analytic interest, is particularly interesting because connects the regularity to the dissipation energy, due to the viscous property of the fluid. In particular Leary proved that for $t \geq \theta \approx \frac{||v_0||_2^4}{\nu^5}$ the weak solution becomes regular in ordinary sense.

In a recent paper we investigate on the possibility to improve the upper bound of instant θ. Actually, employing the energy decay we prove that $\theta \approx \frac{\mathrm{L}^2}{2\nu\gamma^2}\log[\frac{4}{\pi}(\alpha+\beta)||v_0||_2^2]$. So that for small Reynolds numbers R the result by Leray is better. For large Reynolds numbers R our estimate furnishes a logarithmic behavior.

Analysis and Optimal Design of Equilibria in the Vlasov-Poisson System

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Abstract

We investigate the analysis and optimal design of stationary equilibrium distributions for the Vlasov–Poisson system in the presence of an external electric field. Starting from stationary Maxwellian solutions, the kinetic model is reduced to a normalized nonlinear Poisson–Boltzmann equation for the self-consistent electric potential. Existence and uniqueness of the equilibrium potential are established through two complementary approaches: a Schauder fixed-point argument based on uniform estimates for the normalized source term, and a variational formulation based on a strictly convex free-energy functional.

Building on these analytical results, we formulate a unified optimal design framework in which the external electric potential acts as the control. Different design criteria are considered, including an ensemble-type valley-potential functional, quadratic tracking of a prescribed equilibrium density, and the Kullback–Leibler divergence. First-order optimality conditions are derived by means of an adjoint formulation, and a projected nonlinear conjugate-gradient method is employed for the numerical solution of the resulting optimization problems. Numerical experiments illustrate the effectiveness of the proposed approach in shaping and confining equilibrium particle distributions according to different design objectives.

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Algorithms of very high space-time orders of accuracy for hyperbolic equations in the semidiscrete WENO-DeC framework

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In this talk, we investigate a family of arbitrary high-order finite volume methods for hyperbolic partial differential equations. They are based on a semidiscrete approach, in which a Weighted Essentially Non–Oscillatory spatial reconstruction is employed together with a Deferred Correction time discretization, allowing for the construction of schemes of arbitrary high order of accuracy. The methods are tested, up to order 13, on a wide variety of problems of different nature for the linear advection and Euler equations, including smooth problems, tests with strong discontinuities, and long-time evolution problems. The results highlight the computational advantages of adopting very high-order accuracy in space and time [2]. We also examine the influence of the numerical flux within this framework [1], with particular attention to centred fluxes based on simple flux evaluations [3], and further illustrate how insufficiently accurate time discretizations may limit the accuracy of otherwise high-order spatial approximations.

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Relaxation dynamics of open quantum systems: application of the Lindblad formalism to quantum phase space

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We discuss the application of Lindblad theory to the kinetic phase-space formalism to investigate quantum decoherence in particle systems, where interactions with the environment are modeled by Markovian stochastic non-Hermitian operators. Particular emphasis is placed on the analysis and explicit determination of non-Hermitian operators associated with dissipative forms, alongside a rigorous study of the convergence of stochastic models toward Lindblad-type quantum kinetic equations. Furthermore, we present a mathematical study of a Wigner–Lindblad model for a 1D quantum system. Numerical tests indicate the long-time convergence of the solution toward a thermal equilibrium distribution for systems confined in anharmonic traps.

Decoherence effects in the Wigner-Boltzmann formalism

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A quantitative analysis of the electron decoherence is performed in the case where an electron interacts with an environment consisting of a phonon bath at a given temperature. In particular we study the decoherence in terms of the entanglement formation between the electron, initially described by a Gaussian wavepacket, and the environment by using the quantum entropy called Purity, written in terms of the Wigner function. In our work we evaluate, in a rigorous fully quantum mechanical approach, the electron-phonon interaction using the Wigner-function formalism. The problem is numerically solved for by using Monte Carlo simulations. Results are obtained in a one-dimensional GaAs single gaussian well but they can be considered indicative of a more general behavior.

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Transporting Cold Atoms Around Obstacles: A Combined Optimal Control and 4D Phase-Space Approach

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Efficient transport of cold atom ensembles around spatial obstacles is critical for advancing neutral-atom quantum computation and simulation. In this work, we present a two-step computational approach to optimize the two-dimensional transport of neutral Strontium atoms navigating around potential obstacles. Classical optimal control is first employed to derive spatial trajectories that avoid obstacles – modeled as soft penalty terms – while minimizing terminal momentum mismatch. These optimized trajectories then drive a density evolution solver powered by a recently developed open-source 4D phase-space framework for two-level quantum dynamics. We evaluate mass preservation, tweezer potential depth requirements, and boundary condition effects during complex transport protocols, while analyzing the convergence properties and numerical stability of the 4D solver. This work provides a robust methodology to minimize atom loss and decoherence in guided transport setups.

Substitution principles in ideal magneto gas dynamics by means of conditional Lie symmetries

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Substitution principles in unsteady ideal magneto gas dynamics with a separable equation of state are classical results providing new solutions from solutions such that the total magnetic pressure is steady and both velocity and magnetic field are orthogonal to the gradient of a steady differentiable function [1]. In turn, they generalize a similar result in unsteady gas dynamics [2], and older results in steady gas dynamics [3] and steady magneto gas dynamics [4]. Within the framework of Lie conditional symmetries [5], we analyze the equations ruling the flow of an inviscid thermally non-conducting fluid of infinite electrical conductivity in the presence of a magnetic field where external actions are neglected. We prove [6] that, by imposing suitable additional differential constraints, and using Lie infinitesimal methods, it is possible to deduce (in the steady case) and deduce several generalizations (in the unsteady case) of the substitution principles. Moreover, a substitution principle mapping a steady solution of the equations ruling the plane motion of a fluid, with adiabatic index equal to 2 subjected to a transverse magnetic field, to an unsteady solution is presented. A similar approach yields also several substitution principles in ideal gas dynamics [7].

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An L^p-theory for global weak solutions to the Navier-Stokes equations in exterior domains

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We investigate the existence and the partial regularity of weak solutions to the Navier-Stokes initial boundary value problem in exterior domains for initial data that do not have finite energy. In particular, we consider initial data in the Lebesgue spaces L^p, $p \in (2, 3)$. Employing a suitable decomposition of the initial datum as the sum of a "small" L^3 contribution and of a "big" L^2 contribution, we obtain a global weak solution. The solution is constructed as the sum of a global regular solution to an auxiliary Navier-Stokes problem, related to the "small" L^3 contribution to the initial datum, and of a global weak solution to a perturbed Navier-Stokes problem, related to the "big" L^2 contribution to the initial datum. For our weak solution, following the ideas introduced in [1], we prove a partial regularity result in the spirit of Leray's *Théorème de Structure*. Of course, our result holds also in the particular cases of the Cauchy problem and of the initial boundary value problem in a half-space.

The talk is based on the recent work [2].

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New trends in charge and phonon transport in low dimensional structures: the activity at UNICT

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The recent research activity of the group of applied mathematics at the Department of Mathematics and Computer Science of the University of Catania is reviewed. The obtained results can be broadly grouped into the following subjects.

Application of the Maximum entropy Principle (MEP) to 2DEG and simulation of DG-MOSFETs[1]

- formulation of MEP in the presence of subbands;
- limiting energy-transport model and simulation of DG-MOSFET.

Semiclassical transport of charges in graphene

- an optimal control problem with evolution equation given by the Boltzmann equation [2].
- an analysis of uncertain quantification through a particle Galerkin- chaos polynomial method for the Boltzmann equation [3].
- simulation of GFETs [4]

Thermal effects

- phonon transport and macroscopic models.

Quantum transport

- quantum corrected hydrodynamical models from the Wigner equation with a general dispersion relation for electrons, including the several branches of phonons [6, 7].
- modelling based on the Schrödinger equation for charge transport in the ballistic regime, beyond the simple effective mass approximation [8, 9] and simulation of a RTD.

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Well-Posedness and Stability of a Thermoelectromagnetic Model

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We study a mathematical model for the interaction between electromagnetic fields and heat transport in a bounded three-dimensional domain [1]. After establishing the well-posedness of the coupled thermoelectromagnetic system, we analyze the long-time behavior of its solutions. We prove exponential stability for positive definite conductivity and characterize the asymptotic dynamics in the semidefinite case, where solutions approach stationary states [2]. We also identify conditions on the domain and the model coefficients that guarantee strong stability.

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Simulazione numerica diretta di flussi turbolenti su superfici scabre

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The influence exerted by rough surfaces on turbulent flows is of interest in a wide variety of fields, including turbomachinery, river flows, and meteorological applications. The reader is referred to [1] and [2] for thorough reviews of the subject. This study analyses the effect of three-dimensional rough surfaces on the displacement of the logarithmic velocity profile relative to that of a smooth wall, which is known as the roughness function, denoted by ΔU^+. Lengths and velocities scaled in wall units (ν/U_τ and U_τ, respectively) are indicated with a + superscript. Here U_τ is the friction velocity and ν is the kinematic viscosity. Five different surface power spectral density (PSD) shapes have been considered, for each of which several rough Gaussian surfaces were generated by varying the root-mean-square (k_{rms}) of the surface heights. These rough surfaces were used as the bottom surface of a channel where the flow was driven by a constant pressure gradient in order to obtain the desired value of the Reynolds number $R_\tau = U_\tau h/\nu$, where h is the channel depth. The study has been carried out by means of direct numerical simulation (DNS). The continuity and Navier-Stokes equations in dimensionless form (see Equation 1) were solved using centred, second-order finite differences on a staggered grid. The time advancement is based on a third-order Runge-Kutta method for the convective terms and on the Crank-Nicolson scheme for the viscous terms.

$$\frac{\partial u_j}{\partial x_j} = 0, \qquad \frac{\partial u_i}{\partial t} + \frac{\partial u_i u_j}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{1}{R_\tau}\frac{\partial^2 u_i}{\partial x_j \partial x_j} + \delta_{1,i}, \qquad (i, j = 1, 2, 3) \tag{1}$$

In addition to k_{rms}, the effective slope (ES), defined as the spatial average of the absolute value of the streamwise surface slope, is another parameter playing an important role. The Reynolds number was kept constant at 500, while k_{rms}, scaled with h, varied in the range 0.005–0.085 and ES in the range 0.018–1.631. The results show that ΔU^+ increases, exceeding 10, when the PSD includes high wavenumbers. For PSDs characterized by low wavenumbers, ΔU^+ tends to scale with ES, whereas ΔU^+ tends to scale with k_{rms} as the wavenumbers increase. The trend of ΔU^+ as a function of ES for a constant k^+_{rms} shows a monotonic increase with a tendency to asymptote towards a constant value. This behaviour differs from that reported in numerous previous studies, which indicated that ΔU^+ is maximised at $ES \approx 0.3$ and then decreases. This distinctive finding appears to be due to the irregularity of the roughness topology. Further details on this study can be found in [3].

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Nonlinear Schrödinger Equation: Examples and Applications

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The Schrödinger equation, introduced by Erwin Schrödinger more than a century ago, plays a fundamental role in modern physics. Its nonlinear generalizations have subsequently found applications in a wide range of physical contexts.

In this talk, we present some examples and applications of nonlinear Schrödinger-type equations, with particular emphasis on the propagation of solitons. We first consider the propagation of short and ultrashort optical pulses in nonlinear optical fibers with inhomogeneous properties. To describe these systems, we study generalized second- and third-order nonlinear Schrödinger equations whose coefficients depend on both time and the propagation distance [1, 2].

We then discuss an application to heat transport in nanostructures, focusing on the existence and propagation of thermal solitons in nanotubes. This provides an example of how nonlinear wave equations can describe coherent and localized thermal excitations in low-dimensional systems [4].

Another application concerns Bose–Einstein condensates, where nonlinear Schr"odinger-type equations provide a natural framework for describing nonlinear matter-wave dynamics. Under suitable conditions, these equations admit dark soliton solutions, which can be observed, for instance, in elongated (cigar-shaped) trapping potentials [3].

We then discuss a different application in which a fourth-order Schrödinger equation, like in [5], is derived from a generalized de Broglie relation, invariant under a duality transformation involving the Planck length. The resulting equation consists of the standard Schrödinger equation supplemented by a higher-order contribution proportional to the square of the Planck length and the bi-Laplacian operator.

These examples illustrate the versatility of nonlinear and generalized Schrödinger equations as mathematical models for nonlinear phenomena, ranging from optical solitons to fundamental modifications of quantum dynamics.

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The Knudsen Layer in Modeling the Heat Transfer at Nanoscale: Bulk and Wall Contributions to the Local Heat Flux

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Starting from the observation that the influence of the heat carriers' boundary scattering on the heat flux is mainly felt in a narrow zone near the system's boundary, the characteristic dimension of which is of the order of the mean-free path of the heat carriers, we introduce the concept of Knudsen layer in the heat transport at nanoscale, and regard the local heat flux as the final resultant of two different contributions: the bulk heat flux and the wall heat flux.

We therefore propose a theoretical model which accounts for those two contributions developed in the framework of phonon hydrodynamics and in agreement with the second law of thermodynamics.

In steady states we then predict both how the local heat flux behaves, and how the thermal conductivity depends on the characteristic dimension of the system. This analysis is performed both in the case of a nanolayer, and in the case of a nanowire.